

Quaternionic Quantum Particles

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Solutions of quaternionic quantum mechanics (QQM) are difficult to grasp, even in simple physical situations. In this article, we provide simple and understandable free particle quaternionic solutions, that can be easily compared to complex quantum mechanics (CQM). As an application, we study the scattering of quaternionic particles through a scalar step potential. We also provide a general solution method for the quaternionic Schrödinger equation, which can be applied to more sophisticated and physically interesting models.

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I. INTRODUCTION

Quaternionic quantum mechanics (QQM) was conceived by considering complex quantum mechanics (CQM) as a model. However, an important difference between these theories concerns the hermiticity of operators: hermitian operators in CQM and anti-hermitian operators in QQM [1]. At first glance, hermiticity seems to be a major difference between the theories, but it is not so. Anti-hermiticity cannot be considered a true difference between QQM and CQM because the hermitian Schrödinger equation of CQM turns into an equation of anti-hermitian operators simply by multiplying of the whole equation by the complex unit i , and most of the complex hermitian operators are converted to anti-hermitian operators using this procedure. In terms of phenomenology, both theories calculate expectation values of their operators using identical formulas. The anti-hermitian formulation of QQM permits the conservation of the probability density current [1], and this is a positive point. However, there are drawbacks concerning the anti-hermitian QQM formulation, and the breakdown of Ehrenfest's theorem in QQM is a serious problem from a physical standpoint [1–3].

Another disadvantage of the anti-hermitian QQM is the lack of a set of simple solutions. In CQM, sophisticated and physically interesting models are built using a set of simple solutions, which provide the basic understanding of the theory as well. Of course, there are solutions to QQM, and we can quote some of them by way of example [4–16], but they do not have the simplicity that allows them to be compared to either CQM or classical solutions.

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More recently, an alternative QQM formulation [17] has emerged from a quaternionic version of the Aharonov-Bohm (AB) effect [18]. The quaternionic AB-effect has an important difference compared to the usual quantum theories: the momentum operator, and consequently the Hamiltonian operator, do not have a defined hermiticity. A consistent theory has been obtained by redefining the expectation value and the probability current, so that the probability current is conserved in this quaternionic AB-solution. This solution has motivated the development of a quaternionic quantum theory of non-anti-hermitian operators [17], and this theory has the important advantage of a well-defined classical limit; therefore, the Ehrenfest theorem is valid in this framework. For an arbitrary operator \mathcal{O} and an arbitrary quaternionic wave function Ψ , the expectation value is defined in the non-anti-hermitian theory to be

$$\langle \mathcal{O} \rangle = \frac{1}{2} \int dx^3 [\Psi^* \mathcal{O} \Psi + (\Psi^* \mathcal{O} \Psi)^*], \quad (1)$$

where the asterisk denotes the conjugate complex. This expectation value recovers the usual definition when wave functions are complex and the operators are hermitian, consequently generalizing it.

In this article, we further develop this non-anti hermitian theory providing a method for solving the quaternionic Schrödinger equation and obtaining its simplest example: the free particle. This solution has many similarities with the complex wave function, but it also has major differences, mainly the contribution of the pure quaternionic components of wave function to the probability current. The quaternionic solutions have constraints that are unknown in the complex case, and thus, non trivial solutions are harder to find. On the other hand, quaternionic solutions present novel features that are unknown in CQM, like a novel time-dependent solution and the possibility of controlling the direction of propagation through the relative amplitude of the complex and pure quaternionic components of the wave function. We have also studied the scattering of quaternionic particles through a scalar step potential, and the quaternionic particles have higher energies, when compared to the complex case. We stress that the solutions presented herein are simple, and it may be immediately verified that they satisfy the quaternionic Schrödinger equation. Anti-hermitian quaternionic solutions [4–16] are much more complicated and subtle, which reduces their interest and potential applicability. The developed general method for finding quaternionic solutions is harder when compared to the usual methods for solving the Schrödinger equation, but the results obtained are illuminating, and we therefore expect it will inspire further research in this area.

This article is organized as follows: in Sections II and III we solve the quaternionic Schrödinger equation using a novel method where a quaternionic solution is obtained from a previously known complex solution. In Section IV we apply the solution method to find the quaternionic free particle, and a few physical aspects of this solution are discussed in Section V. Section VI describes the scattering of the quaternionic free particle through a scalar step potential, while section VII rounds off the article with our conclusions and future perspectives.

II. TIME-DEPENDENT WAVE EQUATIONS

In this article, we adopt the wave equation

$$\hbar \frac{\partial \Psi}{\partial t} i = \mathcal{H} \Psi, \quad (2)$$

where both the Hamiltonian operator \mathcal{H} and the wave function Ψ are quaternionic. There is a second possibility for (2), which places the complex unit i on the left hand side of (2), so that $\hbar \Psi i \rightarrow \hbar i \Psi$, where Ψ represents the time derivative of Ψ . We will discuss this possibility in an upcoming article, where it can be more conveniently explored. As in the complex case, we separate the variables of the wave function, so that

$$\Psi(x, t) = \Phi(x) \Lambda(t). \quad (3)$$

Φ and Λ are quaternionic functions, and we additionally impose Λ as an unitary quaternion with

$$\Lambda = \cos \Xi e^{iX} + \sin \Xi e^{iY} j, \quad \text{so that} \quad \Lambda \Lambda^* = 1, \quad (4)$$

where Λ^* is the quaternionic conjugate. Of course, Ξ , X and Y are time-dependent real functions and j is the anti-commuting quaternionic complex unit, which obeys $ij = -ji$ and $j^2 = -1$. We adopt the symplectic notation for quaternionic numbers (\mathbb{H}), where $q \in \mathbb{H}$ is written

$$q = z + \zeta j \quad \text{with} \quad z, \zeta \in \mathbb{C}. \quad (5)$$

Λ is already written in symplectic notation (4), and Φ will be expressed in the same terms. An unitary quaternion is the natural generalization of the complex exponential function that is the time-dependent part of a complex wave function, and both functions have oscillatory properties that are desirable in quantum theories. Real exponentials are not deployed in CQM, nor will they be considered here, either. In order to separate the time variable in the wave function, we use (3) and (4) in the wave equation (2), and we further impose

$$\dot{\Lambda} i \Lambda^* = \kappa. \quad (6)$$

The dot denotes a time derivative, and $\kappa = \kappa_0 + \kappa_1 j$ is a quaternionic separation constant with κ_0 and κ_1 complex. Thus, from (6) we get

$$-i \dot{\Xi} \sin 2\Xi - \dot{X} \cos^2 \Xi + \dot{Y} \sin^2 \Xi - \frac{i}{2} \left[\sin 2\Xi e^{i(X+Y)} \right]^* j = \kappa. \quad (7)$$

We separate it into two parts according to the dependence on the complex unit j , and the pure quaternionic part gives

$$\sin 2\Xi e^{i(X+Y)} = \kappa_1 t + C. \quad (8)$$

where C is an integration constant. The sine is finite, and consequently $\kappa_1 = 0$. The simplest solution is thus

$$\Lambda(t) = \Lambda_0 \exp \left[-i \frac{\mathcal{E}}{\hbar} t \right], \quad (9)$$

where \mathcal{E} is the energy and Λ_0 is an unitary quaternionic constant. (9) is simply the CQM time-dependent solution with a constant quaternionic phase. A more general solution is obtained for

$$\dot{\Xi} = 0 \quad \text{and} \quad \dot{X} = -\dot{Y} = -\frac{\mathcal{E}}{\hbar}, \quad (10)$$

so that

$$\Lambda(t) = \Lambda_0 \left\{ \cos \Xi \exp \left[-i \frac{\mathcal{E}}{\hbar} t \right] + \sin \Xi \exp \left[i \left(\frac{\mathcal{E}}{\hbar} t + \tau_0 \right) \right] j \right\}, \quad \dot{\Lambda} i \Lambda^* = \frac{\mathcal{E}}{\hbar}, \quad (11)$$

and τ_0 is a real constant. (11) is an amazingly simple quaternionic result, which recovers the complex time-dependent quantum solution when Λ_0 is complex and $\Xi = 0$, and thus generalizes the complex case. In the next section, we proceed accordingly to find time-independent quantum quaternionic solutions that are simple and new like (11).

III. TIME-INDEPENDENT WAVE EQUATIONS

From the previous section, the time-independent Schrödinger equation is

$$\mathcal{H}\Phi = \mathcal{E}\Phi, \quad (12)$$

and we notice that the hamiltonian operator \mathcal{H} is not supposed to be either hermitian or anti-hermitian, only the energy \mathcal{E} is supposed to be real. We propose the spatial wave function

$$\Phi = \phi \lambda, \quad (13)$$

where λ is a quaternionic function and ϕ is a time-independent complex solution of Schrödinger equation with energy E , so that $\mathcal{H}\phi = E\phi$. Using (12) and (13), we get

$$\phi \nabla^2 \lambda + 2 \nabla \phi \cdot \nabla \lambda = \frac{2m}{\hbar^2} (E - \mathcal{E}) \phi \lambda. \quad (14)$$

We can make further progress decomposing the quaternionic function, such that

$$\lambda = \rho K, \quad \text{where} \quad |\lambda| = \rho, \quad K = \cos \Theta e^{i\Gamma} + \sin \Theta e^{i\Omega} j, \quad \text{and} \quad KK^* = 1; \quad (15)$$

where ρ , Θ , Γ and Ω are real functions. We then turn (14) into

$$\frac{1}{\rho} \left[\left(\nabla + \frac{2}{\phi} \nabla \phi \right) \cdot \nabla \rho \right] K + \frac{2}{\rho \phi} \nabla(\rho \phi) \cdot \nabla K + \nabla^2 K = \frac{2m}{\hbar^2} (E - \mathcal{E}) K. \quad (16)$$

Defining

$$\nabla K = p e^{i\Gamma} + q e^{i\Omega} j \quad \text{and} \quad \nabla^2 K = u e^{i\Gamma} + v e^{i\Omega} j, \quad (17)$$

where

$$\begin{aligned} p &= -\sin \Theta \nabla \Theta + i \cos \Theta \nabla \Gamma, & q &= \cos \Theta \nabla \Theta + i \sin \Theta \nabla \Omega, \\ u &= -\cos \Theta \left(|\nabla \Gamma|^2 + |\nabla \Theta|^2 \right) - \sin \Theta \nabla^2 \Theta + i \left(\cos \Theta \nabla^2 \Gamma - 2 \sin \Theta \nabla \Gamma \cdot \nabla \Theta \right) \\ v &= -\sin \Theta \left(|\nabla \Omega|^2 + |\nabla \Theta|^2 \right) + \cos \Theta \nabla^2 \Theta + i \left(\sin \Theta \nabla^2 \Omega + 2 \cos \Theta \nabla \Omega \cdot \nabla \Theta \right), \end{aligned} \quad (18)$$

we can split (16) into its complex and quaternionic parts, respectively

$$\frac{1}{\rho} \left(\nabla + \frac{2}{\phi} \nabla \phi \right) \cdot \nabla \rho + \frac{2}{\rho \phi} \nabla(\rho \phi) \cdot \frac{p}{\cos \Theta} + \frac{u}{\cos \Theta} = \frac{2m}{\hbar^2} (E - \mathcal{E}) \quad (19)$$

$$\frac{1}{\rho} \left(\nabla + \frac{2}{\phi} \nabla \phi \right) \cdot \nabla \rho + \frac{2}{\rho \phi} \nabla(\rho \phi) \cdot \frac{q}{\sin \Theta} + \frac{v}{\sin \Theta} = \frac{2m}{\hbar^2} (E - \mathcal{E}) \quad (20)$$

After defining,

$$\frac{1}{\rho} \left(\nabla + \frac{2}{\phi} \nabla \phi \right) \cdot \nabla \rho = \mathcal{Z}_0, \quad \frac{2}{\rho \phi} \nabla(\rho \phi) \cdot \frac{p}{\cos \Theta} = \mathcal{Z}_1 \quad \text{and} \quad \frac{2}{\rho \phi} \nabla(\rho \phi) \cdot \frac{q}{\sin \Theta} = \mathcal{Z}_2, \quad (21)$$

where \mathcal{Z}_0 , \mathcal{Z}_1 and \mathcal{Z}_2 are complex functions, we separate (19-20) into real components, so that

$$\Re(\mathcal{Z}_0 + \mathcal{Z}_1) - |\nabla \Gamma|^2 - |\nabla \Theta|^2 - \tan \Theta \nabla^2 \Theta = \frac{2m}{\hbar^2} (E - \mathcal{E}) \quad (22)$$

$$\Re(\mathcal{Z}_0 + \mathcal{Z}_2) - |\nabla \Omega|^2 - |\nabla \Theta|^2 + \cot \Theta \nabla^2 \Theta = \frac{2m}{\hbar^2} (E - \mathcal{E}) \quad (23)$$

$$\Im(\mathcal{Z}_0 + \mathcal{Z}_1) + \left(\nabla - 2 \tan \Theta \nabla \Theta \right) \cdot \nabla \Gamma = 0 \quad (24)$$

$$\Im(\mathcal{Z}_0 + \mathcal{Z}_2) + \left(\nabla + 2 \cot \Theta \nabla \Theta \right) \cdot \nabla \Omega = 0 \quad (25)$$

where $\Re(\mathcal{Z})$ and $\Im(\mathcal{Z})$ are respectively the real and the imaginary components of a complex \mathcal{Z} . Thus, every time-independent complex wave function ϕ that satisfies the Schrödinger equation with real energy E has a correspondent quaternionic time-independent wave function. When multiplied by a quaternionic time-independent function $\lambda = \rho K$, the complex wave function generates the quaternionic wave function $\Phi = \phi \lambda$, which satisfies (21-25) and the quaternionic wave equation (12). To the best of our knowledge, this is the simplest and most general method of finding non-relativistic quaternionic wave functions. In the following sections we will look for the simplest quaternionic functions that satisfy these conditions and ascertain several physical properties.

IV. THE QUATERNIONIC PARTICLE SOLUTIONS

The wave function of a complex quantum particle is represented by a complex exponential, and thus the amplitude of the wave function is constant. In analogy to the complex case, we suppose that the quaternionic radius ρ is constant, and therefore

$$\nabla \rho = 0, \quad (26)$$

In this case, the quaternionic wave function is generated from ϕ through a quaternionic geometric phase. A complete investigation of such a quaternionic Berry phase is interesting enough to be the subject of a separate article, which we will do at a latter date. For our purposes, we further simplify our problem if

$$\nabla \phi \cdot \nabla \Gamma = 0, \quad \nabla \phi \cdot \nabla \Omega = 0, \quad \nabla \phi \cdot \nabla \Theta = 0, \quad (27)$$

and then two possible simple solutions emerge. Let us see the first.

$$\text{A. } \nabla^2 \Theta = 0$$

In this case,

$$\Gamma = \gamma \cdot \mathbf{x} + \Gamma^{(0)}, \quad \Omega = \omega \cdot \mathbf{x} + \Omega^{(0)}, \quad \Theta = \theta \cdot \mathbf{x} + \Theta^{(0)}, \quad (28)$$

with γ , ω and θ constant real vectors and $\Gamma^{(0)}$, $\Omega^{(0)}$ and $\Theta^{(0)}$ real constants. We thus obtain several constraints involving the vector norms,

$$|\gamma|^2 = |\omega|^2, \quad |\gamma|^2 + |\theta|^2 = \frac{2m}{\hbar^2}(\mathcal{E} - E), \quad (29)$$

and orthogonality constraints as well,

$$\theta \cdot \gamma = 0, \quad \theta \cdot \omega = 0, \quad \nabla \phi \cdot \theta = 0, \quad \nabla \phi \cdot \gamma = 0, \quad \text{and} \quad \nabla \phi \cdot \omega = 0. \quad (30)$$

In the same fashion that ϕ is a linear combination of two complex exponentials according to the sign of the exponent, the quaternionic solution has four possibilities, and hence the most general wave function is

$$\begin{aligned} \Phi = \phi(\mathbf{x}) & \left[\left(\cos \Theta e^{i\Gamma} + \sin \Theta e^{i\Omega j} \right) Q_1 + \left(\cos \Theta e^{i\Gamma} + \sin \Theta e^{-i\Omega j} \right) Q_2 + \right. \\ & \left. + \left(\cos \Theta e^{-i\Gamma} + \sin \Theta e^{i\Omega j} \right) Q_3 + \left(\cos \Theta e^{-i\Gamma} + \sin \Theta e^{-i\Omega j} \right) Q_4 \right], \end{aligned} \quad (31)$$

where Q_1 , Q_2 , Q_3 and Q_4 are arbitrary quaternionic constants. We can make ϕ constant, so that $E = 0$, and thus obtain the simplest solution of the case, a truly quaternionic free particle. However, we remember that every complex wave function may generate this kind of quaternionic solution. Furthermore, we stress that (31) is very different from the complex case. The function Θ enables the wave function with a novel oscillation, totally unknown in QQM.

$$\text{B. } \nabla^2 \Theta \neq 0$$

Let us choose

$$\Gamma = \gamma \cdot \mathbf{x} + \Gamma^{(0)}, \quad \Omega = \omega \cdot \mathbf{x} + \Omega^{(0)}, \quad (32)$$

and the vector constraints

$$\nabla \phi \cdot \gamma = 0, \quad \nabla \phi \cdot \omega = 0, \quad \nabla \phi \cdot \nabla \Theta = 0, \quad \nabla \Theta \cdot \gamma = 0 \quad \text{and} \quad \nabla \Theta \cdot \omega = 0. \quad (33)$$

The equations to be solved are

$$|\nabla \Theta|^2 + |\omega|^2 \sin^2 \Theta + |\gamma|^2 \cos^2 \Theta = \frac{2m}{\hbar^2}(\mathcal{E} - E) \quad \text{and} \quad \nabla^2 \Theta + \left(|\gamma|^2 - |\omega|^2 \right) \sin \Theta \cos \Theta = 0. \quad (34)$$

If we apply the gradient operator to the $|\nabla \Theta|^2$ equation, we obtain the $\nabla^2 \Theta$ equation with a changed sign, and consequently $\nabla^2 \Theta = 0$, recovering the previous case. Thus there is no non-trivial solution to this situation.

V. THE FREE QUATERNIONIC PARTICLE

The complex free particle solution enables important quantum models to be developed, such as the infinite well, the finite well, scattering phenomena and wave packets. In the previous section, we saw that this complex wave function has a quaternionic generalization. In this section, we will discuss this mathematical solution in physical terms. Accordingly, we will make use of the probability current defined in [17], namely

$$\mathbf{j} = \frac{1}{2m} \left[\Phi^* \hat{\mathbf{p}} \Phi + (\Phi^* \hat{\mathbf{p}} \Phi)^* \right], \quad (35)$$

and the quaternionic momentum $\hat{\mathbf{p}}$ is defined in [17] as

$$\hat{\mathbf{p}} = -\hbar(\nabla|i), \quad \text{so that} \quad \hat{\mathbf{p}}\Phi = -\hbar\nabla\Phi i. \quad (36)$$

Using (13) and (17), we get the probability current of the quaternionic wave function to be

$$j = \rho^2 \cos 2\Theta j_0 + \frac{\hbar}{m} \rho^2 |\phi|^2 \left(\cos^2 \Theta \nabla \Gamma - \sin^2 \Theta \nabla \Omega \right), \quad (37)$$

where j_0 is the CQM probability current. By way of example, let us calculate the probability current of a quaternionic wave function (31) where $Q_1 = 1$ and $Q_2 = Q_3 = Q_4 = 0$, and the complex wave function is the free particle

$$\phi(\mathbf{x}) = A_1 e^{ik \cdot \mathbf{x}} + A_2 e^{-ik \cdot \mathbf{x}}, \quad \text{where} \quad |k|^2 = \frac{2mE}{\hbar^2}, \quad (38)$$

where A_1 and A_2 are complex constants. From (31) and (37), we get

$$j = \frac{\hbar}{m} \left[\cos 2\Theta \left(|A_1|^2 - |A_2|^2 \right) \mathbf{k} + |\phi|^2 \left(\cos^2 \Theta \nabla \Gamma - \sin^2 \Theta \nabla \Omega \right) \right]. \quad (39)$$

j satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0, \quad (40)$$

and thus there is no gain and no loss of probability in the free particle solution. As expected, the complex result is recovered if $\nabla \Gamma = \mathbf{0}$ and $\Theta = 0$. There is no probability flux along the $\nabla \Theta$ direction, and consequently no momentum is carried along this direction, however, the particle is allowed to move along the $\nabla \Theta$ direction. Along the directions orthogonal to $\nabla \Theta$, the Θ function is a simple parameter of the solution, and it may be made constant without affecting the probability flux and, of course, on the momentum expectation value.

Another feature involves the contributions for the probability flux due to $\nabla \Gamma$ and $\nabla \Omega$. If these vectors are collinear and have a common positive direction, $\nabla \Gamma$ increases j and $\nabla \Omega$ attenuates the flux. This fact may be interpreted in terms of anti-particles that move in the opposite direction of the particle, and this interpretation has been made for relativistic quaternionic solutions [12–14]. However, this may not necessarily be the case. Another interpretation is that $(\cos^2 \Theta \nabla \Gamma - \sin^2 \Theta \nabla \Omega)$ contributes the probability flux of a single particle. The current attenuates and even inverts depending on the relation between the amplitudes of the complex and quaternionic parts of the wave function. This interpretation does not require the existence of anti-particles, and it is in agreement with the complex case. Two simple examples illustrate the situation.

$$\Phi_1 = \cos \Theta e^{ik \cdot \mathbf{x}} + \sin \Theta e^{-ik \cdot \mathbf{x}} j \quad \text{and} \quad \Phi_2 = e^{ik \cdot \mathbf{x}} (\cos \Theta + \sin \Theta j), \quad (41)$$

where Θ is a real constant and k is a real vector. The probability currents are

$$j_1 = \frac{\hbar}{m} \mathbf{k} \quad \text{and} \quad j_2 = \frac{\hbar}{2m} \cos 2\Theta \mathbf{k}. \quad (42)$$

The intensity of j_1 is identical to the intensity of the probability current generated by the complex particle (38) when $A_2 = 0$, and we interpret Φ_1 as a single particle wave function. On the other hand, Φ_2 generates a probability flux whose intensity depends on Θ , and even $j_2 = \mathbf{0}$ if $\Theta = \pi/4$. Accordingly, we can understand j_2 as a single particle probability current, and Θ determines the intensity of the probability flux. Although there is neither probability current nor momentum along the $\nabla \Theta$ direction, the value of the angle affects the direction and the intensity of the flux, and thus Θ is in fact a relevant physical variable whose precise meaning must be determined on a case-by-case basis.

VI. THE STEP POTENTIAL

The quaternionic solutions we examined in the previous section may be written as

$$\Phi = \phi K, \quad (43)$$

where ϕ is a complex wave function and K is a unit quaternion, and can be understood as a complex solution with a quaternionic phase. This kind of solution can hardly generate physically novel solutions because geometric phases generate observable effects only in interaction processes. Conversely, we observed that the single particles (41) present differences compared to the complex cases, even without inter-particle interactions. Let us go further to

observe whether quaternionic effects may happen to single particle systems, like the scattering of quaternionic free particles by the scalar step potential

$$V = \begin{cases} 0 & \text{for } x < 0, & \text{region I} \\ V_0 & \text{for } x \geq 0, & \text{region II,} \end{cases} \quad (44)$$

where V_0 is a real positive constant and the potential V splits the three-dimensional space into two parts bordered by the Oyz plane. We propose the wave function

$$\begin{aligned} \Phi_I &= \cos \Theta_k e^{i(k \cdot x + \gamma_k^\perp \cdot x)} + \sin \Theta_k e^{i(-k \cdot x + \omega_k^\perp \cdot x)} j + R \left[\cos \Theta_q e^{i(-q \cdot x + \gamma_q^\perp \cdot x)} + \sin \Theta_q e^{i(q \cdot x + \omega_q^\perp \cdot x)} j \right] \\ \Phi_{II} &= T \left[\cos \Theta_p e^{i(p \cdot x + \gamma_p^\perp \cdot x)} + \sin \Theta_p e^{i(-p \cdot x + \omega_p^\perp \cdot x)} j \right] \end{aligned} \quad (45)$$

with R and T complex constants and \mathbf{k} , \mathbf{q} , \mathbf{p} , γ_a^\perp and ω_a^\perp real vectors for $a = k, q, p$. We also suppose that Θ_a are constants and adopt that an arbitrary vector \mathbf{v} splits into components according to

$$\mathbf{v} = \mathbf{v}^\parallel + \mathbf{v}^\perp, \quad (46)$$

where \mathbf{v}^\parallel is the component of \mathbf{v} that is parallel to \mathbf{k} and \mathbf{v}^\perp is the component of \mathbf{v} that is normal to \mathbf{k} . Schrödinger's equation permit us to get

$$|\mathbf{k}|^2 + |\gamma_k^\perp|^2 = |\mathbf{q}|^2 + |\gamma_q^\perp|^2 = \frac{2m}{\hbar^2} \mathcal{E} \quad \text{and} \quad |\mathbf{p}|^2 + |\gamma_p^\perp|^2 = \frac{2m}{\hbar^2} (\mathcal{E} - V_0), \quad (47)$$

where it has been used that

$$|\gamma_a^\perp|^2 = |\omega_a^\perp|^2 \quad \text{for} \quad a = k, p, q. \quad (48)$$

There is a set of boundary conditions at the point of incidence $\mathbf{x}_0 = (0, y_0, z_0)$, but we can set $\mathbf{x}_0 = (0, 0, 0)$ without loss of generality. Considering the continuity of the wave function,

$$\Phi_I(\mathbf{x}_0) = \Phi_{II}(\mathbf{x}_0) \quad \Rightarrow \quad \begin{cases} \cos \Theta_k^{(0)} + R \cos \Theta_q^{(0)} = T \cos \Theta_p^{(0)} \\ \sin \Theta_k^{(0)} + R \sin \Theta_q^{(0)} = T \sin \Theta_p^{(0)} \end{cases} \quad (49)$$

$$\nabla \Phi_I^\parallel(\mathbf{x}_0) = \nabla \Phi_{II}^\parallel(\mathbf{x}_0) \quad \Rightarrow \quad \begin{cases} \mathbf{k} \cos \Theta_k^{(0)} - R \mathbf{q} \cos \Theta_q^{(0)} = T \mathbf{p} \cos \Theta_p^{(0)} \\ -\mathbf{k} \sin \Theta_k^{(0)} + R \mathbf{q} \sin \Theta_q^{(0)} = -T \mathbf{p} \sin \Theta_p^{(0)}. \end{cases} \quad (50)$$

Considering \mathbf{k} , \mathbf{q} and \mathbf{p} collinear vectors, we obtain

$$|T|^2 = \frac{|\mathbf{k} + \mathbf{q}|^2}{|\mathbf{p} + \mathbf{q}|^2} \quad \text{and} \quad |R|^2 = \frac{|\mathbf{k} - \mathbf{p}|^2}{|\mathbf{p} + \mathbf{q}|^2}. \quad (51)$$

We obtain the simplest solution imposing real coefficients R and

$$|\mathbf{k}| = |\mathbf{q}|. \quad (52)$$

Furthermore, (47) requires

$$|\gamma_k^\perp|^2 = |\gamma_q^\perp|^2. \quad (53)$$

We notice that $\gamma_a^\perp = \mathbf{0}$ recovers the probability density of the complex case, but the wave function is still quaternionic. A complex limit is only recovered if $\Theta_a = 0$, and we conclude that the wave function (45) generalizes the complex case because the physical results of the complex case are recovered within a limit, even though the wave function is still quaternionic. We can hypothesize that complex solutions may have a quaternionic counterpart with identical physical predictions. Yet, the analysis of the quaternionic step demands the boundary conditions along the \mathbf{k}^\perp direction

$$\nabla \Phi_I^\perp(\mathbf{0}) = \nabla \Phi_{II}^\perp(\mathbf{0}) \quad \Rightarrow \quad \begin{cases} \gamma_k^\perp \cos \Theta_k^{(0)} + R \gamma_q^\perp \cos \Theta_q^{(0)} = T \gamma_p^\perp \cos \Theta_p^{(0)} \\ \omega_k^\perp \sin \Theta_k^{(0)} + R \omega_q^\perp \sin \Theta_q^{(0)} = T \omega_p^\perp \sin \Theta_p^{(0)}. \end{cases} \quad (54)$$

To finally solve the problem, let us suppose that the γ_a vectors are collinear, and so are the ω_a vectors. We stress that γ_a^\perp and ω_a^\perp are not necessarily collinear, although they have identical magnitudes. We also remember that R and T satisfy the CQM relation

$$|k| - |q|R = |p|T. \quad (55)$$

Comparing (54) with (55), we obtain

$$\frac{|\gamma_q| \cos \Theta_q^{(0)}}{|\gamma_k| \cos \Theta_k^{(0)}} = \frac{|\omega_q| \sin \Theta_q^{(0)}}{|\omega_k| \sin \Theta_k^{(0)}} = -1 \quad \text{and} \quad \frac{|\gamma_p| \cos \Theta_p^{(0)}}{|\gamma_k| \cos \Theta_k^{(0)}} = \frac{|\omega_p| \sin \Theta_p^{(0)}}{|\omega_k| \sin \Theta_k^{(0)}} = \frac{|p|}{|k|}. \quad (56)$$

(56) permits us say that

$$\sin^2 \Theta_k^{(0)} = \sin^2 \Theta_q^{(0)} = \sin^2 \Theta_p^{(0)}. \quad (57)$$

and thus,

$$\frac{|p|^2}{|k|^2} = \frac{|\gamma_p^\perp|^2}{|\gamma_k^\perp|^2} = 1 - \frac{V_0}{\mathcal{E}}. \quad (58)$$

The (58) relation, between the incoming and transmitted momenta, is equivalently obeyed in the complex case, and thus the quaternionic particle (45) is possibly the simplest quaternionic generalization of the complex scattering. The solution depends only on the parameters of the incident particle: the energy \mathcal{E} , the transverse momentum γ_k and on the intensity of the scalar potential V_0 and Θ_k angle. We observe that all the components of probability j are collinear, but the flux is not necessarily normal to the Oxy -plane. The direction of the incident probability flow is determined by Θ_k , γ_k and ω_k , while the only effect of V_0 is the intensity of the transmitted momentum p . The potential does not change the direction of the transmitted and reflected particles. This means that the system does not behave like a light beam, and consequently does not satisfy some version of the Snell law. This remark is important because this a behavior has been observed in anti-hermitian QQM [19], and the reasons for this difference must be investigated.

VII. CONCLUSION

In this article we presented a general method for finding quaternionic quantum solutions. The quaternionic time-dependent wave function generalizes the CQM result with a unitary quaternion, whereas starting points of the time-independent solution are CQM-wave functions ϕ that generate quaternionic solutions when multiplied to a quaternion function λ , and hence the quaternionic solutions are such that $\Phi = \phi\lambda$. The solution method does not suppose hermiticity for operators, and thus the results are out of the main stream of QQM, which is mainly anti-hermitian. Our approach, however, has the advantage of a well-behaved classical limit, something not accomplished within the anti-hermitian framework.

The method has been applied to obtain the simplest quantum solution: the free particle. The quaternionic free particle has a limit whose physical properties are identical to the complex quantum free particle. However, the wave function has novel oscillations, and this is evidence that our approach must be considered as an alternative quaternionic generalization of quantum mechanics.

The scattering of a quaternionic particle through a scalar step potential has also presented many similarities with the complex case. The parameters of the quaternionic case may regulate the intensity and direction of the probability flow, something unobserved in the complex case. The solution is very simple compared to the anti-hermitian quaternionic cases, for example [9], and then we hope that this simplicity will inspire further research in the field.

We can outline several perspectives for future research. Many mathematical questions that are currently studied in anti-hermitian QQM [20] can be addressed to the non-anti-hermitian formalism used in the present article. On another side, throughout the text we have observed that there is a second possibility to the wave equation (3), where i is placed on the left hand side of Ψ , and also the study of quaternionic geometric phases, which have already been started with the quaternionic AB-effect [18], but that may deserve a more specific treatment. In principle, every result of quantum mechanics is at risk of being revised using the non-anti-hermitian formalism, and therefore, the field of research is vast. We hope that it can be thoroughly investigated in the future.

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